# IMPURITY DYNAMICS IN A BOSE CONDENSATE

Siu A. Chin and Harald A. Forbert

Center for Theoretical Physics and Department of Physics Texas A&M University, College Station, TX 77843 USA

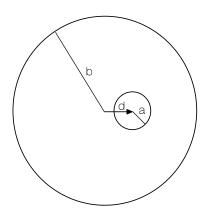
## 1. INTRODUCTION

Bose-Einstein condensation is the macroscopic occupation of a single quantum state. In bulk liquid Helium, most theoretical calculations[1] agree that, in the limit of zero temperature, roughly 10% of the Helium atoms are condensed in the ground state. For recently observed atomic condensates in <sup>87</sup>Rb [2], <sup>7</sup>Li [3] and <sup>23</sup>Na [4], nearly 100% condensation is expected because of their low density. This collective occupation essentially magnifies ground state properties by a factor N equal to the number of condensed atoms. For macroscopic  $N \approx 10^{24}$ , this exceedingly large factor can be exploited to detect minute changes in the condensate ground state. Thus aside from its intrinsic interest, BEC is potentially a very sensitive probe.

In this work, we will explore changes in the condensate ground state induced by a "sizable" impurity. By "sizable", we mean an impurity whose size is within a few orders of magnitude of the trap size, and not necessarily atomic in scale. A sizable impurity will "drill" a hole in the condensate wave function and alter its energy. The question is whether this microscopic change can be detected macroscopically because of the Bose-Einstein condensation effect. This is described in the next section. We discuss the effects of interaction in Section 3 and the case of two or more impurities in Section 4.

## 2. IMPURITY EXPULSION

The effect we seek to describe is generic. We will therefore consider the problem in its simplest conceptual context. We imagine a non-interacting Bose gas of mass m confined to a spherical cavity (an infinite square well) of radius b. We introduce an impurity, which to first order approximation, can be regarded as a hard sphere of radius a. When the impurity is placed inside the cavity, the wave function of the Bose gas must vanish on the surface of both the cavity and the hard sphere. Since the cavity only serves to confine the Bose gas, it may or may not also trap the impurity.



**Figure 1.** The Bose gas is confined in a spherical cavity of radius b and excluded from an off-center impurity, which is a hard sphere of radius a.

Classically, since there is no interaction between the cavity and the hard sphere, the hard sphere is free to be anywhere inside the cavity. However, when the cavity is filled by a Bose gas, the position of the impurity is dictated by the ground state energy of the Bose gas. Thus there is a quantum mechanically induced interaction between the hard sphere and the cavity.

The situation is as shown in Fig. 1, where the hard sphere is displaced by a distance d from the cavity center. The impurity is assumed to be sufficiently massive that the Born-Oppenheimer approximation is adequate. The effective potential for the impurity is then just  $V(d) = NE_0(d)$ , where  $E_0(d)$  is the ground state energy of a single particle confined in a spherical cavity with an off-center hole:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) = E(d)\psi(\mathbf{r}), \qquad \psi(\mathbf{r}) = 0 \quad \text{at} \quad |\mathbf{r}| = a \quad \text{and} \quad |\mathbf{r} + \mathbf{d}| = b. \quad (1)$$

When d = 0, both the ground state wave function and the energy are known analytically

$$\psi_0(r) = \frac{1}{r} \sin\left[\frac{\pi(r-a)}{(b-a)}\right],\tag{2}$$

$$E_0 = \frac{\hbar^2}{2m} \frac{\pi^2}{(b-a)^2}.$$
 (3)

When the impurity is off-center, spherical symmetry is broken and the problem is non-trivial. Instead of solving the problem exactly, we gauge this off-center effect by a variational calculation using the following trial function

$$\phi(\mathbf{r}) = \left(1 - \frac{a}{r}\right)(b - |\mathbf{r} + \mathbf{d}|). \tag{4}$$

The first factor is the zero energy solution (Laplace's equation) satisfying the Dirichlet condition at  $|\mathbf{r}| = a$ . The second factor forces the wave function to vanish at the

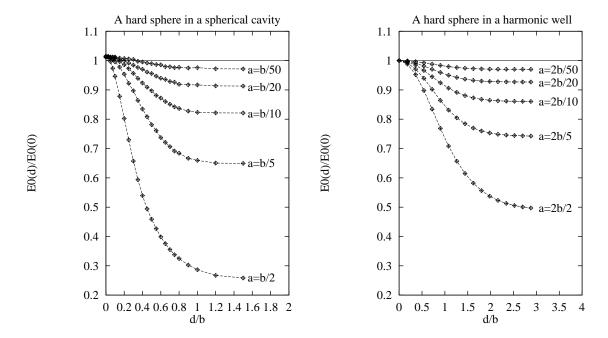


Figure 2. Left: The ground state energy of a particle in a spherical cavity of radius b with a displaced hard sphere of radius a. The energy as a function of the displacement for various impurity sizes is normalized by dividing by the exact on-center energy. Right: Similar calculations for the case of an impurity in a harmonic well. In this case b is the harmonic length and the energy is only normalized by dividing by the variational on-center energy. In both cases, the impurity is not assumed to be trapped by the cavity or the well.

displaced cavity surface. For d=0, the resulting variational energy simply replaces the factor  $\pi^2$  in (3) by 10, which is an excellent approximation. For finite d, the resulting energies are as shown in Fig. 2. The angular integration is sufficiently cumbersome that we computed the variational energy by the method of Monte Carlo sampling. The energy is lower as the impurity moves off center. This result is easy to understand once one has seen it. The impurity "drills" a hole in the cavity's ground state wave function. It is more costly to drill a hole near the wave function's maximum (the center) than at its minimum (the edge). Thus a sizable impurity will be expelled by a Bose condensate.

Similar results are obtained if one replaces the spherical cavity by a spherical harmonic oscillator. The size parameter b can be identified as the harmonic length via

$$\hbar\omega = \frac{\hbar^2}{m} \frac{1}{b^2}.\tag{5}$$

The harmonic oscillator ground state wave function is then

$$\psi_0(\mathbf{r}) = \exp\left[-\frac{1}{2}\left(\frac{r}{b}\right)^2\right]. \tag{6}$$

When an impurity is placed in this harmonic well, the ground state wave function is again altered. We now do a variational calculation with the trial function

$$\phi(\mathbf{r}) = \left(1 - \frac{a}{r}\right) \exp\left[-\frac{1}{2}\left(\frac{|\mathbf{r} + \mathbf{d}|}{\alpha}\right)^{2}\right],\tag{7}$$

where  $\alpha$  is a variational parameter. The angular integral can be done exactly when we displace the harmonic oscillator rather than the impurity. The remaining radial integral can then be computed by numerical quadrature. The results are also shown in Fig. 2. In order to compare this with the cavity case, we must take at least 2b, and not just b, as the equivalent cavity radius. Since the exact on-center energy in this case has no simple analytic form, we normalize by dividing by the variational on-center energy.

To get an order-of-magnitude estimate of the expulsion force, consider the case of lithium atoms with  $\frac{\hbar^2}{m} \approx 7$  K Å<sup>2</sup> and  $b \approx 3 \times 10^4$  Å. The characteristic energy scale is

$$\hbar\omega = \frac{\hbar^2}{m} \frac{1}{b^2} \approx \frac{7}{(3 \times 10^4)^2} \approx 10^{-8} \text{K}.$$

The variation in energy is over some fraction of the trap radius. Thus the expulsion force due to each atom is

$$F \approx \frac{10^{-8} \text{K}}{10^4 \text{Å}} \approx \frac{10^{-8} \text{K} \, 10^{-13} \text{J/K}}{10^4 \text{Å} \, 10^{-10} m/\text{Å}} \approx 10^{-25} \text{ Newton.}$$

For  $N \approx 10^{24}$  Bose condensed atoms, the expulsion force IS macroscopic. Currently, the maximum N achieved in any of the atomic trap experiment is only about  $10^6$ . Such a small force may still be detectable if the impurity is sufficiently light.

## 3. THE EFFECT OF INTERACTION

To gauge the effect of interaction among the Bose condensed atoms, we do a variational Hartree calculation. For interacting Bosons confined in a harmonic well, the Hamiltonian is

$$H = \frac{\hbar^2}{2m} \sum_{i} (-\nabla_i^2 + \frac{r_i^2}{b^4}) + \sum_{i>j} v(\mathbf{r}_{ij}).$$
 (8)

In the low density limit, the two-body potential can be replaced by the scattering length approximation

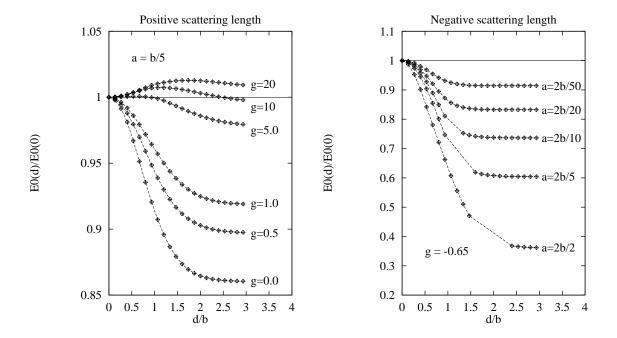
$$v(\mathbf{r}_{ij}) \to 4\pi \frac{\hbar^2}{m} a_{sc} \delta^3(\mathbf{r}_{ij}).$$
 (9)

For a Hartree wave function consisting of a product of normalized single particle states  $\phi(\mathbf{r}_i)$ 

$$\Psi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_n) = \prod_{i=1}^n \phi(\mathbf{r}_i), \tag{10}$$

the variational energy is given by

$$\frac{E_V}{N} = \frac{\hbar^2}{2m} \left[ \int d^3r \phi(\mathbf{r}) (-\nabla^2 + \frac{r^2}{b^4}) \phi(\mathbf{r}) + (N-1) 4\pi a_{sc} \int d^3r \phi^2(\mathbf{r}) \phi^2(\mathbf{r}) \right]. \tag{11}$$



**Figure 3.** Left: The change in energy at one impurity size a = b/5 as a function of the interaction strength  $g = Na_{sc}/b$ . Right: The change in energy for various impurity sizes at one negative interaction strength g = -0.65. Variationally, the system would collapse at g = -0.67 without any impurity. The straight segments correspond to impurity locations that would destabilize the condensate.

Minimizing this with respect to  $\phi(\mathbf{r})$  yields the Gross-Pitaevskii equation. To account for the hard sphere impurity, one must again require  $\phi(\mathbf{r})$  to vanish on the impurity's surface. Instead of solving this problem exactly, we simply take

$$\phi(\mathbf{r}) = \frac{1}{\sqrt{Z}} \left( 1 - \frac{a}{|\mathbf{r} + \mathbf{d}|} \right) \exp\left[ -\frac{1}{2} \left( \frac{r}{\alpha} \right)^2 \right], \tag{12}$$

where Z is the normalization integral, and minimize the energy functional (11) with respect to the parameter  $\alpha$ . This is in the spirit of using Gaussian trial wave functions to study the Gross-Pitaevskii equation, as suggested by Baym and Pethick [5] in the context of BEC.

The interaction is characterized by a strength parameter  $g = Na_{sc}/b$ . The left panel of Fig. 3 shows the effect for positive scattering length. For g < 5, the results are only slightly higher than those in the last section. All atomic experiments are far below the g = 5 limit. In the extreme case of  $g \ge 10$ , the picture changes completely and the impurity is stabilized at the center. However, when the effective interaction is this strong, the mean-field approximation is no longer creditable and one must consider two-body correlations, as in the case of liquid Helium.

The effect of negative scattering length is shown on the right panel of Fig. 3. Variationally, as shown by Fetter [6], the condensate by itself is unstable below g < -0.67. When g is close but above this critical value, the introduction of a

sufficiently large impurity will cause the the condensate to collapse. This is shown by the straight line segements on Fig. 3. For these locations of the impurity, there are no energy minima for the variational parameter  $\alpha$ . When the impurity is at the center, it increases the single particle energy and there is no collapse. However, as it moves off center, the energy is lowered and the condensate collapses. This is also understandable from the opposite direction; when g is close to the critical value, as the impurity enters the condensate, it increases the condensate density without substantially increasing the single particle energy. It pushes g over the critical value and the condensate collapses.

### 4. TWO OR MORE IMPURITIES

For the case of n impurities, each having a different radius  $a_i$  and located at  $\mathbf{d}_i$ , one can simply generalize the single particle trial function (12) to

$$\phi(\mathbf{r}) = \frac{1}{\sqrt{Z}} \prod_{i=1}^{n} f_i(\mathbf{r}) \exp\left[-\frac{1}{2} \left(\frac{r}{\alpha}\right)^2\right], \tag{13}$$

with

$$f_i(\mathbf{r}) = \left(1 - \frac{a_i}{|\mathbf{r} + \mathbf{d}_i|}\right). \tag{14}$$

The resulting expression for the variational energy has a simple form

$$\frac{E_V}{N} = \frac{\hbar^2}{m} \left[ \frac{3}{2} \frac{1}{\alpha^2} + \frac{1}{2} \left\langle \sum_{i=1}^n \mathbf{g}_i^2 - \left( \sum_{i=1}^n \mathbf{g}_i - \frac{\mathbf{r}}{\alpha^2} \right)^2 + \frac{r^2}{b^4} \right\rangle \right],\tag{15}$$

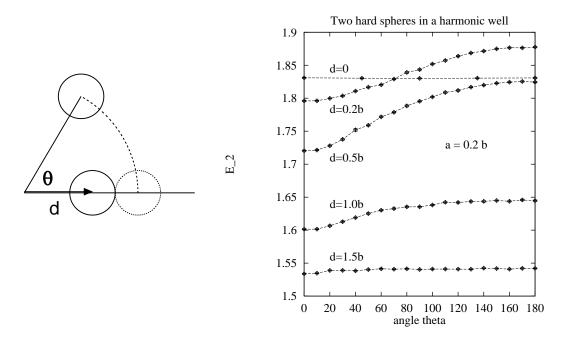
where

$$\mathbf{g}_i = \frac{\nabla f_i}{f_i},\tag{16}$$

and the expectation value is with respect to the trial function (13). The first two terms in the expectation value involving  $\mathbf{g}_i$  may be interpreted as the kinetic energy of each impurity and their collective interaction with the harmonic well. With more than one impurity, there is no way to do the angular integration exactly. We evaluated the expectation value in (15) by the Monte Carlo method.

For n=2, the resulting energy  $E_2=E_V/\hbar\omega$  is shown in Fig. 4. In order to disentangle the two-impurity interaction energy from the effect of off-center energy dependence, we separate the two impurities by keeping each at equal distance from the trap center. The configuration used is as shown on the left panel of Fig. 4. The resulting energy on the right panel clearly shows that there is an effective attraction between the two impurities. This is induced by the Bose condensate. It is less costly to "drill" a slightly larger hole at one place than to "drill" two separated holes. One can therefore infer that multiple impurities tend to clump together and will be expelled from the trap center.

The effect of interaction can again be assessed by including a Gross-Pitaevskii type mean-field interaction. For the present qualitative discussion, we have not bothered to include this correction.



**Figure 4.** Left: Two impurities maintaining the same distance from the harmonic well center while rotating through an angular separation  $\theta$ . Right: The energy for two impurities, each of size a = 0.2b, as a function of angular separation at various distances from the well center.

## 5. CONCLUSIONS

In this work, we have considered the possible use of BEC as a sensitive probe for detecting microscopic changes in the condensate ground state. Our variational studies suggest that

- a) A hard-sphere-like impurity will be expelled from the center of a condensate. For a light but sizable impurity, such an expulsion maybe macroscopically observable.
- b) A sizable, hard-sphere-like impurity will accelerate the collapse of a condensate with negative scattering length.
- c) A Bose condensate induces an effective attraction among hard-sphere-like impurities. This may have interesting implications for induced dimerization or clusterization of weakly interacting impurities, such as <sup>3</sup>He.

Work is currently in progress to seek exact solutions for problems that have only been solved variationally in this work.

#### ACKNOWLEDGMENTS

This research was funded, in part, by the U.S. National Science Foundation

grants PHY95-12428 and DMR-9509743 (to SAC). The idea of impurity expulsion was evolved from considerations of impurity delocalization in Helium droplets[7-9]. The latter was first suggested by my colleague and collaborator E. Krotscheck.

## REFERENCES

- [1] R. M. Panoff and P. A. Whitlock, in *Momentum Distribution*, edited by R. N. Silver and P. E. Sokol, Plenum Publishing, 1989.
- [2] M. H. Anderson et al., Science **269**, 198 (1995)
- [3] C. C. Bradley et al., Phys. Rev. Lett. **75**, 1687 (1995); **78**, 985 (1997)
- [4] K. B. Davis et al., Phys. Rev. Lett. **75**, 3969 (1995)
- [5] G. Baym and C. Pethick, Phys. Rev. Lett. **76**, 2477 (1996)
- [6] A. L. Fetter, "Ground State and Excited States of a confined Bose Gas," cond-mat/9510037.
- [7] E. Krotscheck and S. A. Chin, Chem. Phys. Lett. **227**, 143 (1994).
- [8] S. A. Chin and E. Krotscheck, Phys. Rev. B52, 10405 (1995)
- [9] S. A. Chin and E. Krotscheck, *Recent Progress in Many-Body Theories*, Vol. 4, P.85, edited by E. Schachinger *et al.*, Plenum Press, 1995.